

BIAS-FREE ESTIMATION IN MULTICOMPONENT MAXIMUM LIKELIHOOD FITS WITH COMPONENT-DEPENDENT TEMPLATES

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The possibility of strong biases in a multicomponent Maximum Likelihood fits with component-dependent templates has been demonstrated in some toy problems. We discuss here in detail a problem of practical interest, particle identification based on time-of-flight or dE/dx information. We show that large biases can occur in estimating particle fractions in a sample if differences between the momentum spectra of particles are ignored, and we present a more robust fit technique, allowing bias-free estimation even when the particle spectra in the sample are unknown.

1. Introduction

It has been shown in some toy problems¹ that strong biases may occur in a multicomponent Maximum Likelihood fit whenever the templates, i.e. the functions, used to parameterize the probability distributions used in the fit are not fixed but depend on event observables. An interesting example of such a problem in the practice of experimental High Energy Physics is the statistical separation of different kinds of particles on the basis of limited-precision measurements of particle-dependent quantities, like Time-of-Flight or energy loss (dE/dx).

2. Particle Fractions estimation

Consider a sample of particles generated by a certain physical process in our experiment. We know that the given sample is a mixture of known particle types, for example *Pions*, *Kaons* and *Protons*, but unfortunately we don't know the fractions of each type, respectively indicated by f_π , f_K , f_P . Let's assume that our experimental apparatus includes a Particle Identification (*PID*) device, providing the measurement of some quantities whose distribution depends on the particle type. Using this *PID* information we want to estimate f_π , f_K and f_P , by means of an Unbinned Maximum Likelihood fit of our data sample.

The above problem is very common in particle physics, for example it occurs in separating different decay modes of a given particle³ (same final state multiplicity and topology but different final state

particle types), in studies of fragmentation of heavy quarks², or in optimizing the performances of algorithms for tagging the flavor of *B* mesons².

We will consider two common methods for particle identification: one is based on the measurement of energy loss of charged particles due to the ionization of a gas or of a semiconductor (often the same device used to measure particle momentum), the so called dE/dx measurement; the other is based on the measurement of the Time-of-Flight (*TOF*) of the particle. A common feature of *PID* devices based on the above principles is that the separation power between different particles is not a constant, but strongly depends on the momentum of the given, unknown, particle. A clear example of this feature is shown in Fig 1 where the dE/dx mean response of different particles is plotted as a function of momentum in the drift chamber of a typical High-Energy Physics experiment. Assuming that the resolution of the measurement is constant, the separation power dramatical changes in a short momentum range. As a consequence of the dependence of the mean value of the *PID* response on the particle momentum, the templates describing the *PID* variable's *p.d.f.* are not fixed but depend, on an event-by-event base, on the momentum of the particle: we clearly are in the situation described in¹ where the templates of the fit depend on a component of the fit itself.

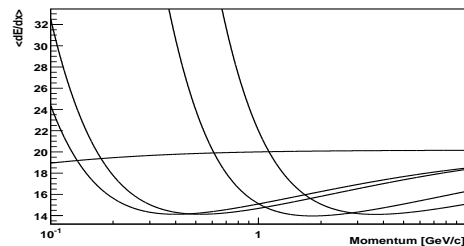


Fig. 1. The mean value of the energy loss of charged particles as a function of the momentum in a typical experiment.

2.1. The Likelihood expression

Consider, for simplicity, only the PID information provided by a dE/dx measurement. Our observables are then the dE/dx (pid) and the momentum of the track (mom). We will indicate as $type$ the particular particle hypothesis. Unfortunately, we cannot simply write the Likelihood function as:

$$L(f_j) = \prod_i \left(\sum_{j=\pi, K, P} f_j P(pid_i | mom_i, type_j) \right). \quad (1)$$

Using expression (1) may give a strongly biased result if our additional variable, the momentum, has different distributions depending on the particle type (see next section). As discussed in¹, whenever the templates used in a multi-component fit depend on additional observables, to avoid the bias it is necessary to use the correct, complete Likelihood expression, including the explicit distributions of all observables for all classes of events. In our case, the above implies that we need to include in our Likelihood the momentum distributions of each particle type. We should also notice that in practice those distributions are almost always different.

We then write the correct Likelihood function as:

$$\begin{aligned} L(f_j) &= \prod_i \left(\sum_{j=\pi, K, P} f_j P(pid_i, mom_i | type_j) \right) \quad (2) \\ &= \prod_i \left(\sum_{j=\pi, K, P} f_j P(pid_i | mom_i, type_j) \right. \\ &\quad \left. \times P(mom_i | type_j) \right), \end{aligned}$$

with the condition:

$$\sum_{j=\pi, K, P} f_j = 1. \quad (3)$$

3. A toy study

We generated a sample of different particle types with known composition as follow:

- PID variable is distributed, for each particle, according to a typical resolution function (i.e. the template used in the fit) defined as:

$$PID_{\text{measured}} - PID_{\text{expected}}(mom) \quad (4)$$

Note the dependence on momentum of the expected PID .

It is important to note that we have chosen typical realistic values for all needed parameters.

This distribution represents:

$$P(pid_i | mom_i, type_j) \quad (5)$$

in Eq. (2).

- Momenta of the particles are distributed according a Gaussian $N(\mu_j, \sigma_j)$, where $j = \pi, K, P$ and:

$$\mu_\pi = 1.00, \quad \mu_K = 1.25, \quad \mu_P = 1.25,$$

$$\sigma_\pi = \sigma_K = \sigma_P = 0.50.$$

Those distributions obviously represent:

$$P(mom_i | type_j) \quad (6)$$

of equation 2.

- Particle fractions where fixed to:

$$f_\pi = 50\%, \quad f_K = 35\%, \quad f_P = 15\%.$$

We then used an unbinned Maximum Likelihood fit to estimate the particle fractions of the sample using the Likelihood function described in Eq. (2) where:

$$P(mom_i | type_j) = N(\mu_j, \sigma_j). \quad (7)$$

In Fig. 2 (upper plot) the distribution of the estimators for f_π and f_P are shown for thirty toy samples of ten thousand particles each. As expected, the fractions returned by the fit are well centered on the true values given by the input.

Conversely, the same distributions obtained with the incomplete Likelihood function of Eq. (1) (Fig. 2, lower plot) are affected by a bias much larger than the nominal statistical uncertainty of those measurements, due to the difference in the momentum distribution of each particle type. This demonstrates that the effect predicted in¹ is actually very significant in real-life problems of Particle Identification.

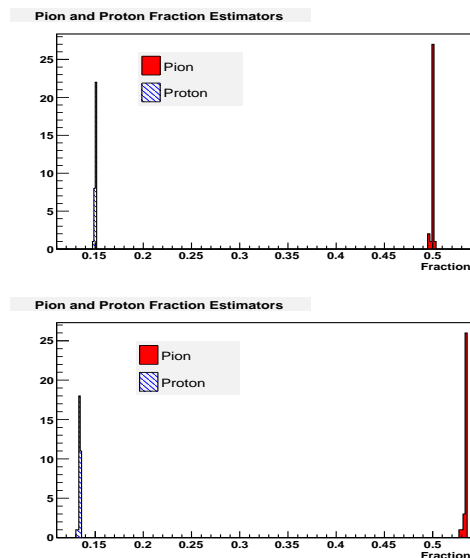


Fig. 2. The Pion and Proton fraction estimator distributions when the complete (top) and incomplete (bottom) Likelihood expression is used.

3.1. The case of unknown momentum distributions

Writing the complete Likelihood function considering the distribution of all the observables used in the fit is relatively straightforward in principle.

On the other hand, in practice, we often have poor information about those distributions; sometimes they are completely unknown. It is the case, for example, of the particle fractions produced during the fragmentation of heavy quarks where the corresponding momentum distributions are unknown and no functional hypothesis can be made.

Considering what was shown in the previous section, we now wonder how to avoid the bias and write the complete Likelihood if the additional observable distributions are unknown.

If no specific functional form can be assumed, we may want to use a general one, e.g. we could consider a Series Expansion as a description of the distributions with the expansion coefficients left as free parameters to be determined by the fit.

We then write the momentum term of the Likelihood function (2):

$$P(mom_i, type_j) = \sum_m a_{mj} U_m(mom_i) \quad (8)$$

where m is the order and U_m are the basis vectors used for the series expansion.

Coming back to our toy sample, we considered Orthogonal Polynomials as a basis for the expansion. Amongst a number of possibilities, we selected Second Type Chebyshev Polynomials (denoted by U_m).

We then replaced in expression (2) the term Eq. (7) with Eq. (8) and we performed again the unbinned Maximum Likelihood Fit, this time by fitting also the parameters of the polynomial expansion. As shown in Fig. 3, now the bias is brought back to zero, as it was when we assumed perfect knowledge of the individual momentum distributions of each particle type. We have been able to avoid the bias in

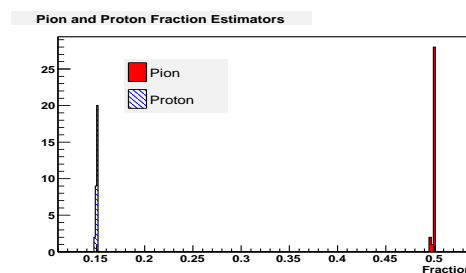


Fig. 3. The Pion and Proton fraction estimator distributions using a Series Expansion as a parameterization of the momentum distribution.

the fraction fit, without any particular assumption on the functional form of the momentum distributions. In such a way we simulated the practical case where no information is known about the additional observable distributions. Please notice also that just the first seven terms of the Second Type Chebyshev Expansion were needed in order to parametrize each particle type momentum distribution. Another interesting aspect is that comparing Fig. 3 to Fig. 2 no significant degradation in the resolution of the estimator is observed, although the number of parameters is increased. In Fig. 4 the projections of the fit to the toy sample are shown.

3.2. A more complicated case: Time of Flight

Suppose that our *PID* information is obtained by the measurement of the Time of Flight. The expression of the expected TOF is a function of two observables:

$$TOF_{\text{expected}}(mom, L) = \frac{L/c}{\sqrt{1 + (m_j/mom)^2}} \quad (9)$$

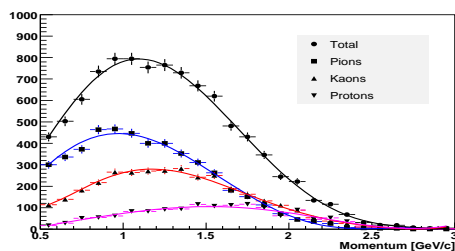


Fig. 4. The momentum projections for each particle type superimposed on the corresponding generated distributions.

where L is the length travelled by the particle during its time measurement (arclength) and it is a function of the production angle of the particle (in the cylindrical geometry of the TOF detector), c is the speed of light, m_j is the mass of the particle hypothesis j and mom is again the momentum. Both the momentum and the arclength distributions could be different for each particle type, i.e., both observables could be source of bias in the particle fractions estimation. Assuming no correlations between the momentum and the arclength, we have to modify the expression (2) to be:

$$\begin{aligned}
 L(f_j) &= \prod_i \left(\sum_{j=\pi,K,P} f_j P(pid_i | mom_i, arc_i | type_j) \right) \\
 &= \prod_i \left(\sum_{j=\pi,K,P} f_j P(pid_i | mom_i, type_j) \right. \\
 &\quad \times P(mom_i | type_j) \\
 &\quad \times P(arc_i | type_j) \left. \right).
 \end{aligned}$$

We then added the simulation of the arclength in our toy sample according to a normal distribution $N(\mu_j, \sigma_j)$ using the values:

$$\mu_\pi = 90, \quad \mu_K = 100, \quad \mu_P = 110,$$

$$\sigma_\pi = \sigma_K = \sigma_P = 25.$$

Considering again the case where no information is available about the distributions of each particle type, we used the same technique of the Series Expansion for both variables. We repeated our fit on thirty toy samples and also in this case, as shown in Fig. 5, no bias was observed for our estimator. It is also interesting to observe that we used just three terms of the Chebyshev Expansion for the arclength parameterization, that results in an approximate description of data (see arclength projections in Fig. 6) but it doesn't affect the results of the fit.

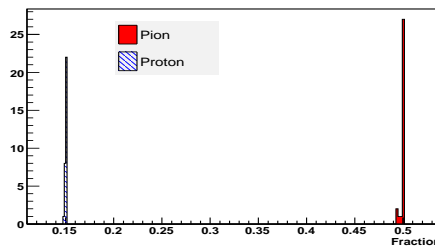


Fig. 5. The Pion and Proton fraction estimator distributions using two Series Expansions as a parameterization of the momentum and the arclength distributions.

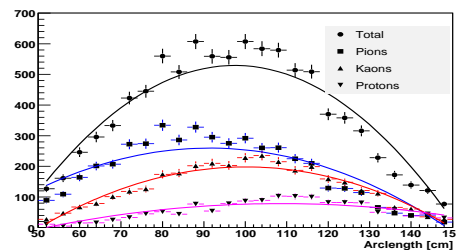


Fig. 6. The arclength projections for each particle type superimposed on the corresponding generated distributions.

4. Conclusions

In this short paper we focused on a practical and common problem of particle physics: the estimation of the particle type fractions using Particle Identification information. We showed that a significant bias can arise from the use of an incomplete expression of the Likelihood under realistic conditions. We also considered a practical problem where no information was assumed about an observable. We eliminated the bias by using Series Expansions of the unknown distributions in orthogonal polynomials, where the coefficients of the expansions are free parameters determined by the fit. We also considered a more complicated example where two relevant observables have unknown distributions, and also in this case the Series Expansion was successful in avoiding biases in determining the fractions of each component.

References

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